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Example 5

Computational Details:

[0085] All calculations were performed using the different modules implemented in the Materials Studio V6.

[0086] The Monte-Carlo methods were used to obtain the most probable locations of the Li species within the low-energy configuration of the COF. These were carried out using the Simulated Annealing techniques available within the Materials Studio V.6.0. Default parameters were utilized. Automatic temperature control and 100000 cycles/cell was employed to optimize the structure. Universal force filed (UFF) in conjugation with a QEq charge equilibration method was employed for the geometry optimization, however, it was noticed that applying the equilibration (QEq) did not make much of a difference to the final configurations. No constraints were placed during the optimizations.

[0087] For the geometry optimization of the periodic COF structure, tight-binding Density Functional Theory was employed. The PBE exchange-correlation functional and parameters from the Slater-Koster library were used with a plane wave basis set cut-off of 340 eV. All calculations were spin polarized and only the Γ-point was sampled. UFF-based Lennard-Jones dispersion corrections were included in Energy, Force and Displacement calculations and the cell was optimized. A smearing parameter of 0.005 Ha was applied.

[0088] To establish the room temperature stability of the lithiated CON a CASTEP dynamics calculation employing a NVE ensemble at 298K was carried out. For the MD simulations, the CASTEP Dynamics module of the Materials Studio was used. For the calculations a 1×1×2 cell was used and the gradient-corrected exchange correlation were applied using the Generalized Gradient Approximation (GGA) and Perdew-Burke-Ernzerhof (PBE) functional. The Newtonian equations of motions (NPT) were chosen for defining the ensemble considering its suitability in optimi-

zation of periodic 2D structure. Ultrasoft pseudopotentials with a plane wave basis cut-off of 260 eV were employed. And, a DFT-D based semi-empirical dispersion correction was applied in the optimization. Electronic minimization was carried out using the Density Mixing functional. Excellent convergence was achieved for all electronic levels and with no noticeable systematic shifts in energy. Tolerance used: 1×e-006.

[0089] The band structures were calculated the geometry optimized configurations (lowest energy configuration from the DFTB) using the CASTEP built within the MS package. For these, a Norm-conserving pseudopotentials with a plane wave basis cut-off of 500 eV was employed and the B3LYP functional was used. Electronic minimizations were achieved using an All Bands/EDFT algorithm. All calculations were performed on the unit cell and separately on a 2×2×2 super cell.

[0090] For the calculation of the electron density and the electrostatic potentials DMol3 implemented in the Materials Studio was employed. For the calculations a 2×2×2 cell was used and the gradient-corrected exchange correlation were applied using the Generalized Gradient Approximation (GGA) and Perdew-Wang 91 (PW91) functional. A DFT-D correction was applied, a Global scheme was used for the orbital cut-off (5.1 Ang.) with a SCF tolerance of 1×e-006. And a smearing parameter of 0.005 Ha was applied.

We claim:

1. Self-exfoliated covalent organic framework derived nanosheets (CONs) with good stability and high porosity comprising plurality of 3,5-diaminotriazole units and plurality of triformyl phloroglucinol units, in extended layered covalent framework wherein, the triazole based diamine units are bonded to the triformyl phloroglucinol units via Schiff bonds to generate a porous structure.

2. The covalent organic nanosheets as claimed in claim 1, wherein the covalent organic nanosheet has the structure of Formula I, and forms channels with pores having dimensions of 1.4 nm×1.7 nm.

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